Comparison of Ambient Measurements to Emissions Representations in Modeling

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Presented to:
The CCOS Technical Committee
Sacramento, CA
October 20, 2005

Background

- Generally, preliminary photochemical modeling results in the San Joaquin Valley (SJV):
  - Underpredict peak, observed ozone concentrations
  - Do not meet model performance metrics in the southern SJV

Project Objective

To provide corroborative evidence, with sufficient justification, that can potentially explain disagreements between modeled and observed pollutant concentrations.

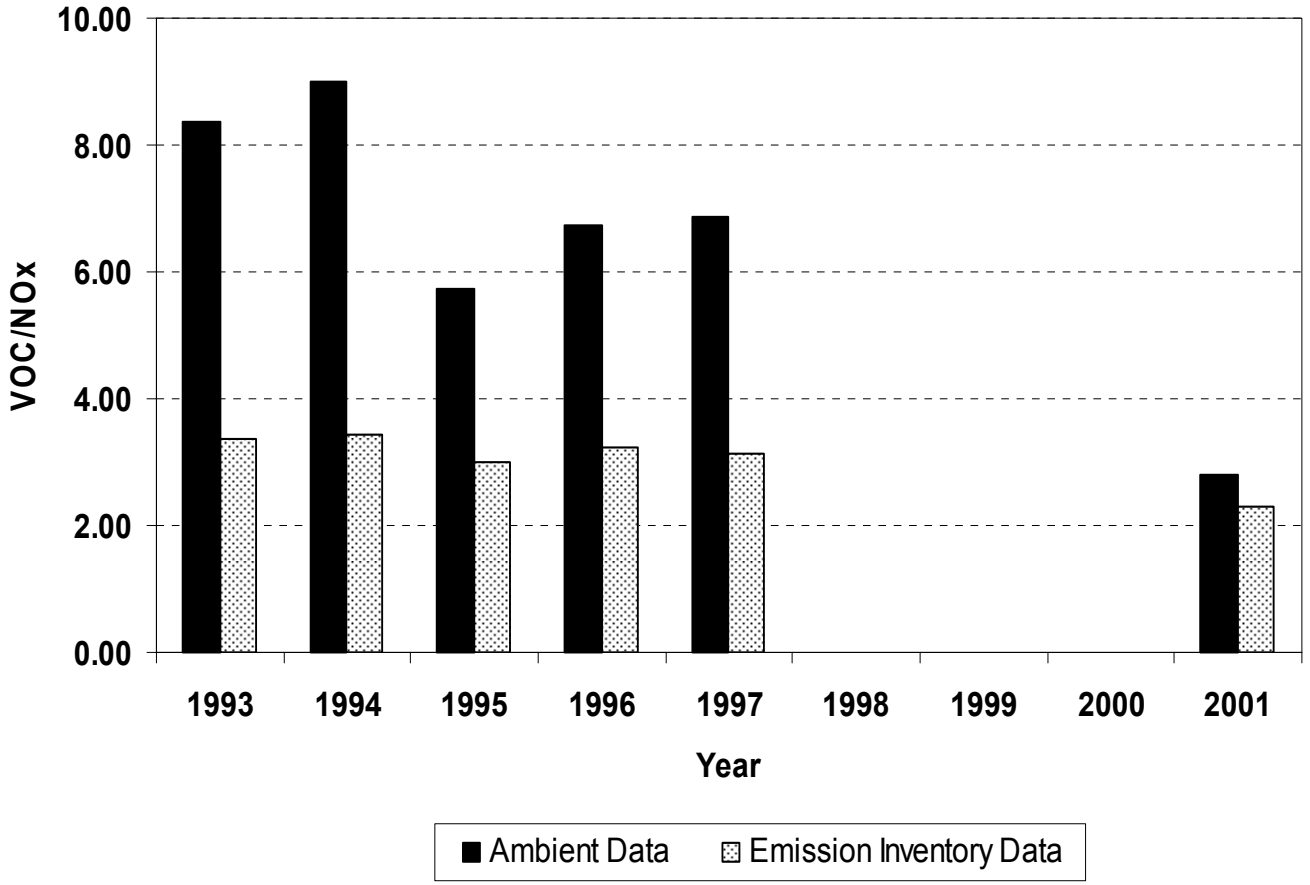
Proposed Techniques (1 of 3)

- Analysis methods
  - Speciation profile review
  - Ratio comparisons (VOC-to-NO_x and individual species)
  - Fingerprint analysis
  - Source apportionment (e.g., CMB and PMF)

CMB = chemical mass balance

PMF = positive matrix factorization

Proposed Techniques (2 of 3)



Emission inventory- and ambient-derived VOC/NO_x ratios at Los Angeles North Main during summer mornings.

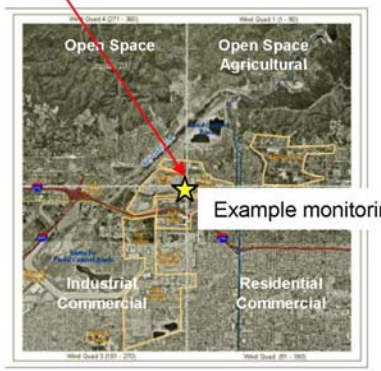
Proposed Techniques (3 of 3)

- Emission inventory (EI) issues to be addressed
  - Spatial allocation
  - Temporal allocation
  - Chemical speciation

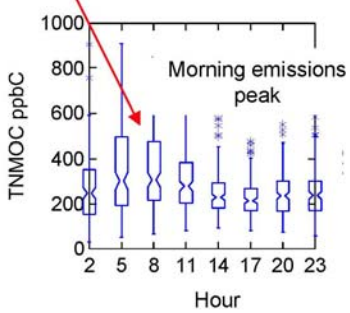
Examples (1 of 4)

Step 1 – Ambient site selection and characterization of a monitoring site.

(a) Site maps are created to help characterize potential emissions influences on each site selected for the analysis.

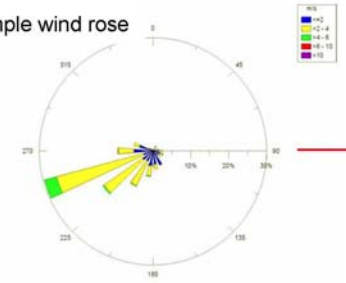


(b) Ambient data are validated and analyzed to determine if a site is influenced by fresh emissions and if data are sufficient for analysis.



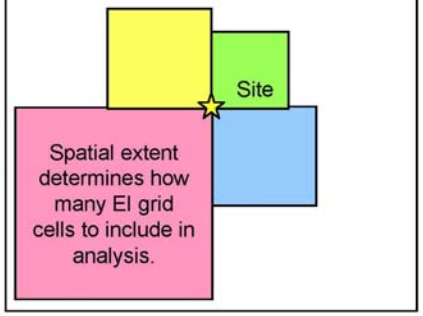
(c) Meteorological data are analyzed to determine predominant wind speed and direction and spatial extent for analysis.

Example wind rose



(d) Spatial extent of the analysis area based on predominant wind speed and direction.

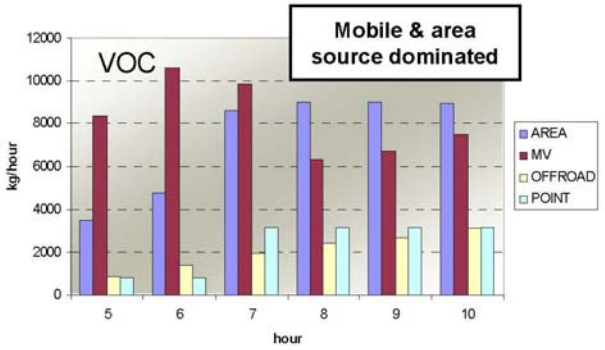
Example spatial extents of analysis region.



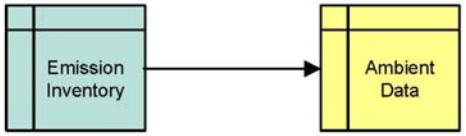
Examples (2 of 4)

Step 2 – Assess and process emission inventory data.

(a) Analyze emission inventory for morning hours and gridded spatial extent determined in Step 1d.

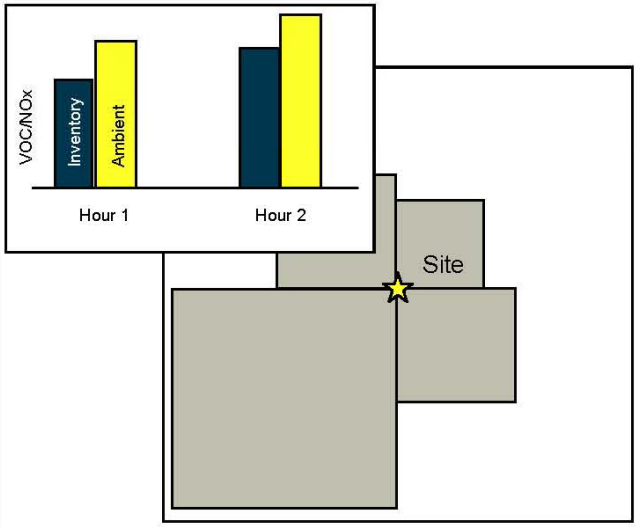


(b) Match VOC species in inventory to species measured at monitoring sites; convert mass to moles for comparison.

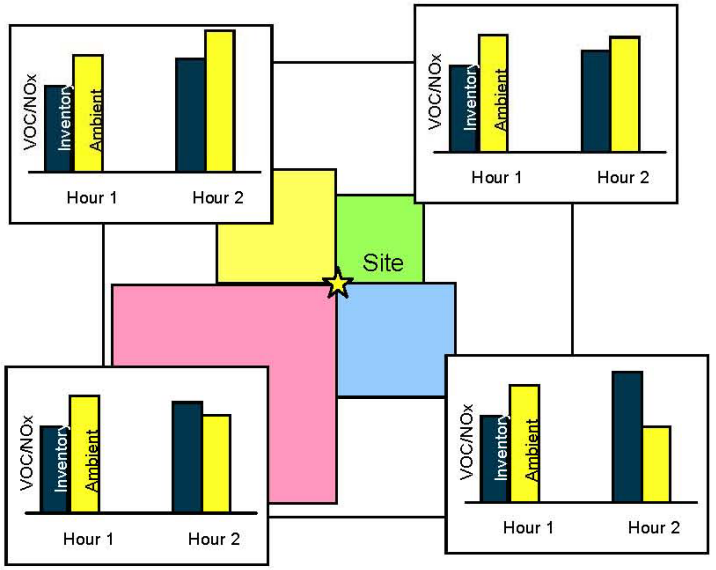


Examples (3 of 4)

Step 3 – Spatial and temporal comparison of VOC/NO_x and CO/NO_x ratios in the ambient data and the emission inventory

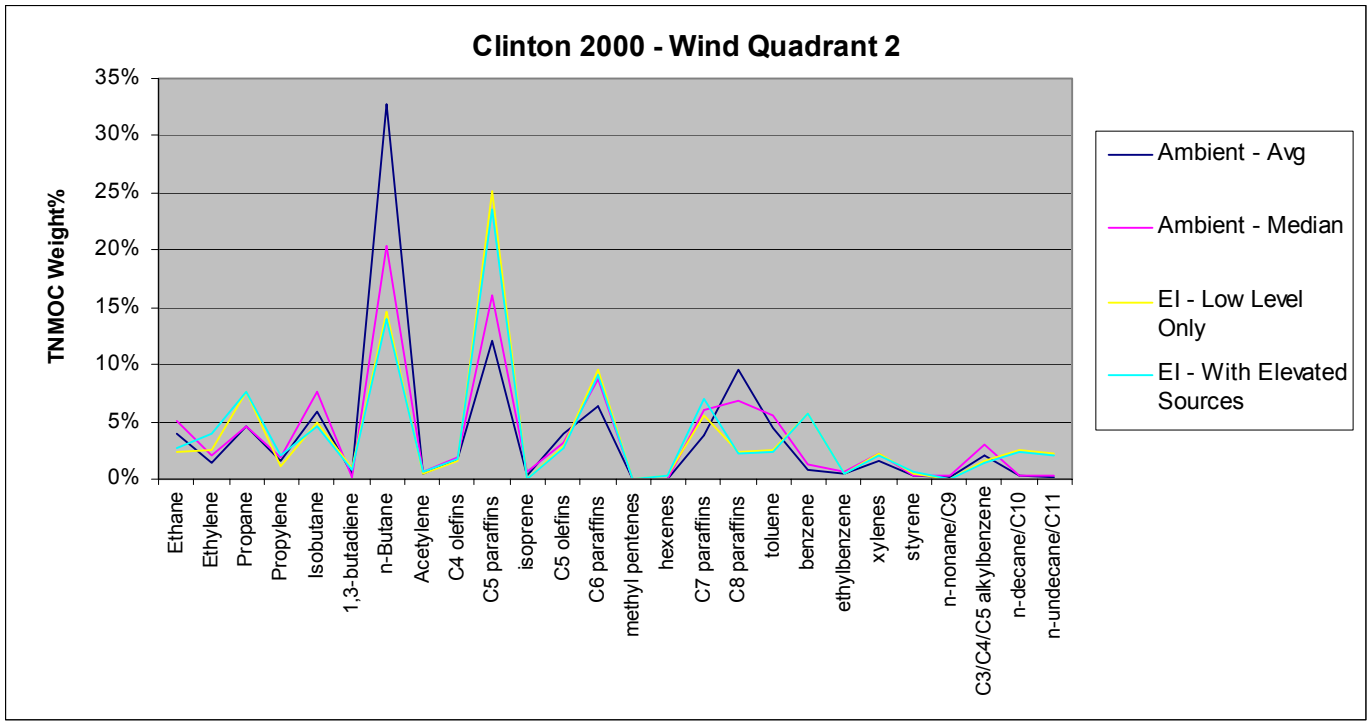


(a) Pollutant ratios are calculated for the entire grid analysis region in the emission inventory and compared to ambient pollutant ratios. Ratios are calculated for the morning time period because emission rates are high, mixing heights are low, and photochemical reaction rates and transport are minimized.



(b) Pollutant ratios are calculated for the morning time period by wind sector to examine how well the emission inventory compares to the ambient data at higher spatial resolutions.

Examples (4 of 4)



Houston Area EI Reconciliation

Spike in ambient concentrations of n-butane when winds were from the southeast.

Speciation profiles for chemical manufacturing plants are likely underestimating this species.

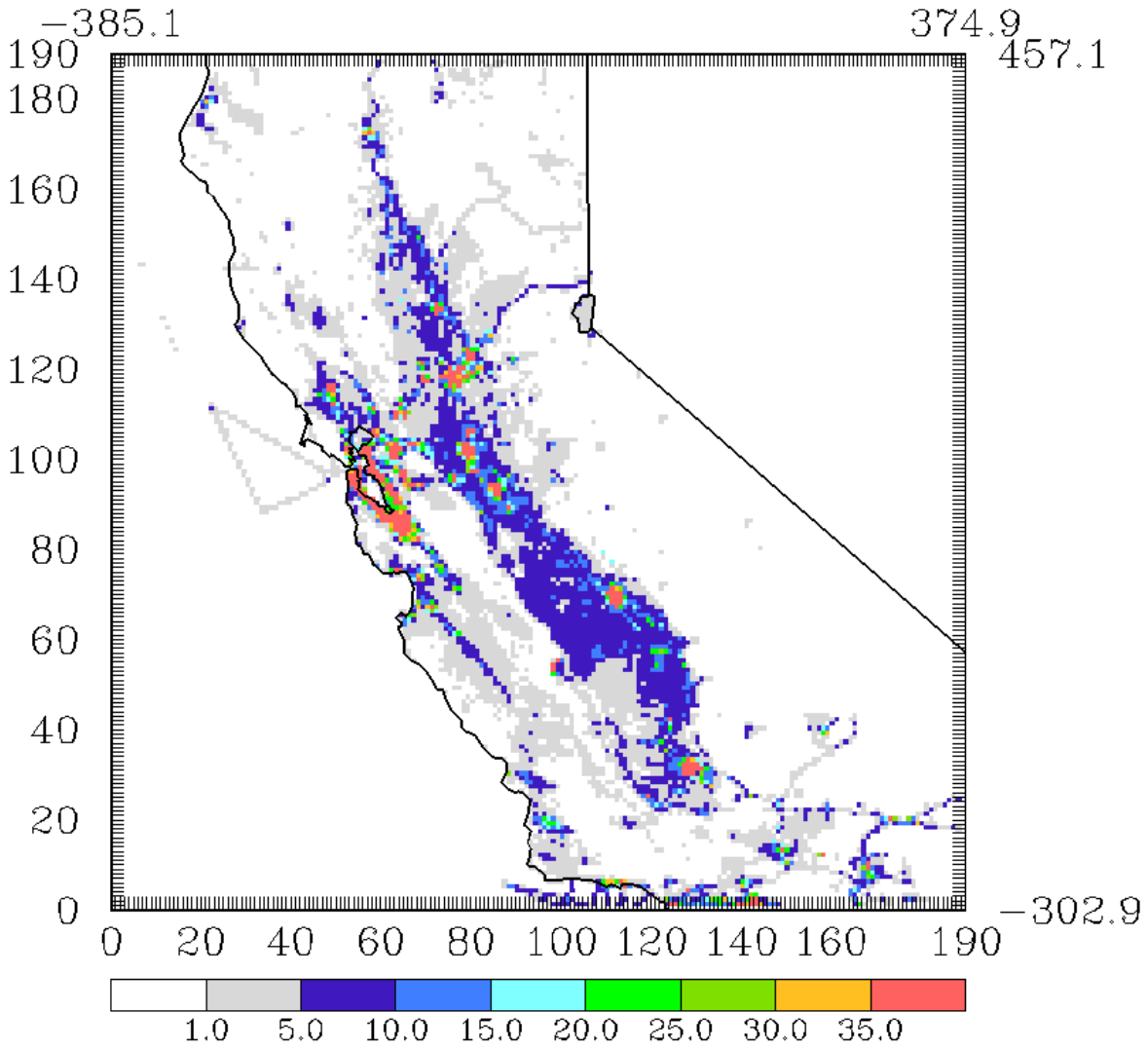
Technical Issues (1 of 5)

- EI specifications
  - Spatially, temporally, and chemically resolved
  - Weekday and weekend day emissions
  - Emissions for VOC, CO, NO_x, and individual chemical species (not grouped by chemical mechanism)

Technical Issues (2 of 5)

Area source NO_x emissions

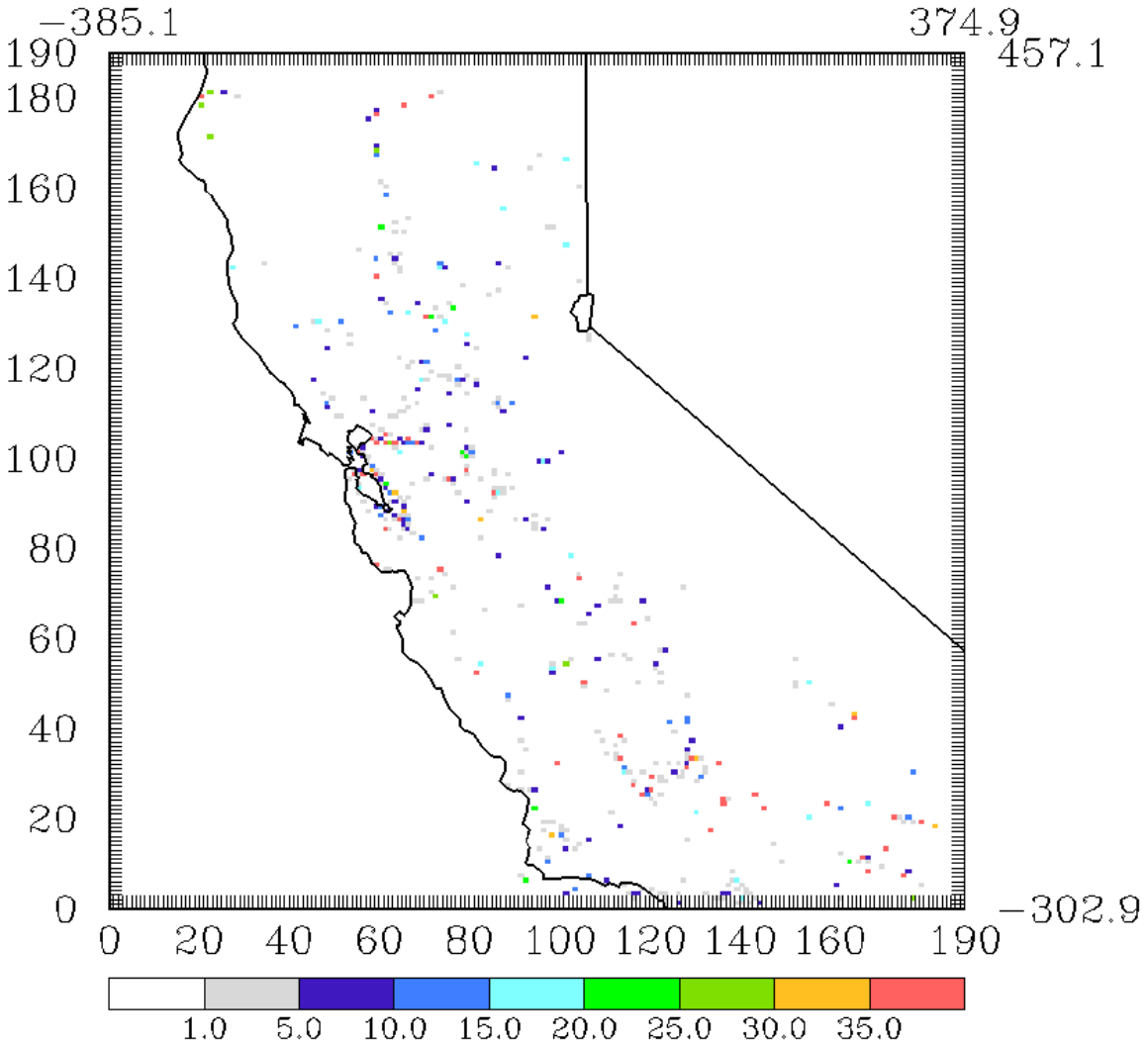
July 31, 2000
12:00 PM



Technical Issues (3 of 5)

Point source NO_x emissions

July 31, 2000
12:00 PM



Technical Issues (4 of 5)

- Ambient data issues
  - Ambient concentrations should exceed a meaningful threshold
  - Ambient data must be representative of nearby emission sources
    - Monitoring sites should be in areas with high emission rates
    - Data should be available during morning hours when mixing heights and photochemical reaction rates are low
    - Elevated sources may or may not impact a monitor

Technical Issues (5 of 5)

- Ambient data issues (continued)
  - Temporal distribution of the data (1-hr or 3-hr data needed)
  - Weekday and weekend day data needed
  - VOC, NO_x, and CO data needed

Statement of Work – Phase 1

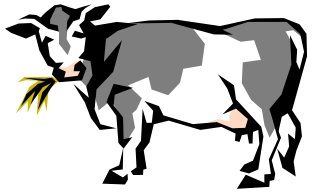
- Task 1 – Kickoff meeting, workplan, and EI data and EI documentation gathering
- Task 2 – Identify available air quality data
- Task 3 – Review ARB chemical speciation profiles
- Task 4 – Evaluate alternative data analysis methods and hold workshop

Task 1 – Gather Emissions Data (1 of 2)

- Work with ARB to acquire Placeholder Modeling EI inputs (e.g., raw county-level by source category and facility) and results (prior to lumped chemical mechanism) currently used by ARB
  - Used for preliminary 1-hr ozone modeling
  - Based on latest data
  - Gross adjustments applied, primarily to approximate updates to EMFAC and OFFROAD

Task 1 – Gather Emissions Data (2 of 2)

- Work with ARB to acquire an improved EI (by the end of Phase 1):
  - Livestock waste



  - Speed/VMT data (EMFAC)

  - Locomotives

  - Vegetation layers in BEIGIS

Task 2 – Identify Available Air Quality Data

Site selection based on

- Data availability (VOC, NO_x)
- Site monitoring objectives
- Ambient concentration levels
- Spatial distribution of sites
- Temporal distribution of the data

Map of Central California air quality monitoring sites

Task 3 – Review Speciation Profiles (1 of 2)

ARB profile for gas-fired external combustion boilers

Profile#	SAROAD	Chemical Name	TOG Fraction
3	43105	ISOMERS OF HEXANE	0.01
3	43122	ISOMERS OF PENTANE	0.09
3	43201	METHANE	0.56
3	43204	PROPANE	0.04
3	43212	N-BUTANE	0.09
3	43220	N-PENTANE	0.06
3	43248	CYCLOHEXANE	0.01
3	43502	FORMALDEHYDE	0.08
3	45201	BENZENE	0.04
3	45202	TOLUENE	0.02

Task 3 – Review Speciation Profiles (2 of 2)

Examine profiles based on

- Associated emissions and reactivity
- Profile age
- Number and quality of underlying source tests
- Applicability to California

Task 4 – Evaluate Alternative Data Analysis Methods

Determine analyses to be conducted during the study's second phase

- Document foundations of the updated CCOS gridded EI
- Prepare technical memo
- Organize one-day workshop
- Decision point for Phase 2

Potential Phase 2 Analyses

- Integrate the results of previous research
- Perform EI reconciliation with pollutant ratios (VOC/NO_x, CO/NO_x)
- Perform EI reconciliation with speciated VOCs (ratios, TNMOC composition)
- Perform VOC source apportionment (e.g., factor analysis, CMB, PMF)

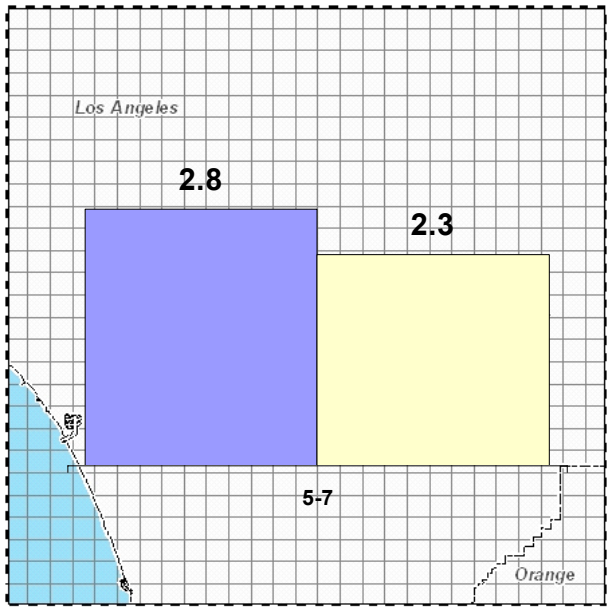
Discussion of Potential Analyses (1 of 6)

Previous and Ongoing Analyses

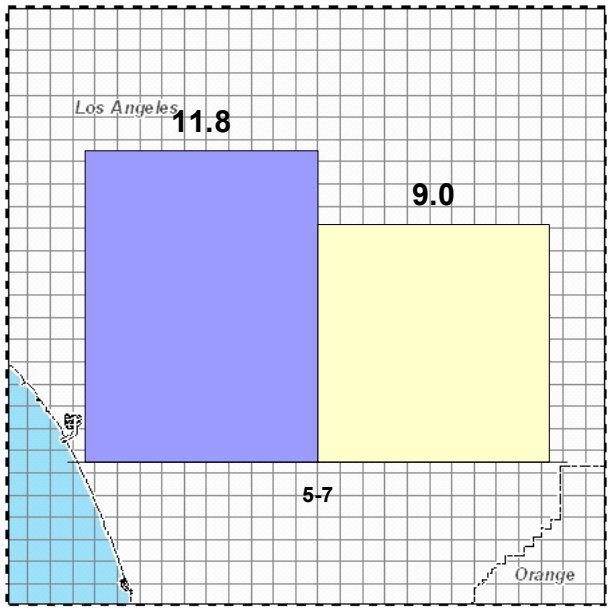
- CCOS modeling studies
  - Tesche et al., 2004 (EI underpredicts VOC reactivity)
  - STI, ongoing (model aloft performance)
- CRPAQS emission reconciliation
  - STI, 2005 (VOC emissions were within 50% in Fresno)
- SCAQMD emission reconciliation
  - STI, 2004 (adjustments to EI were needed to improve temporal distribution of on-road mobile source emissions)
- PAMS data in California
  - STI, 1999 (emission reconciliation showed EI was underestimated by a factor of ~2)

Discussion of Potential Analyses (2 of 6)

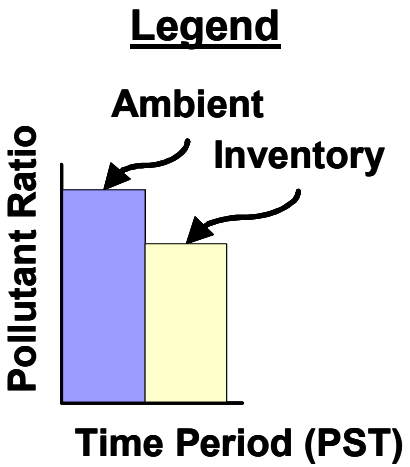
EI Reconciliation with Pollutant Ratios



PAMS HC/NO_x



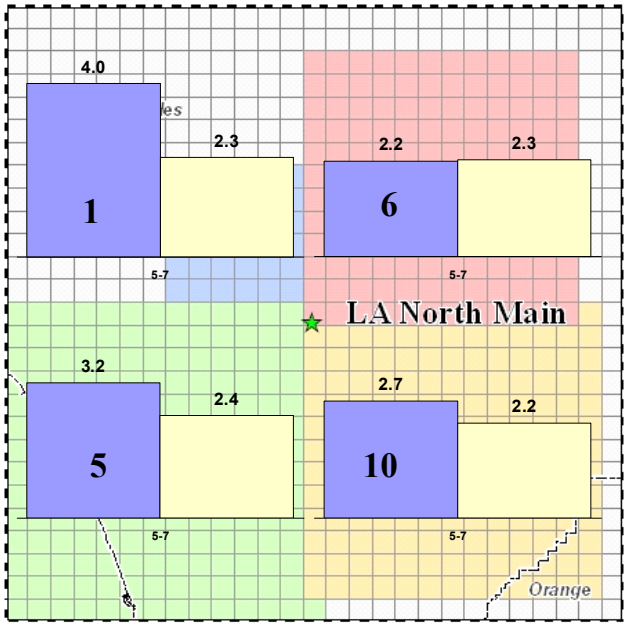
CO/NO_x



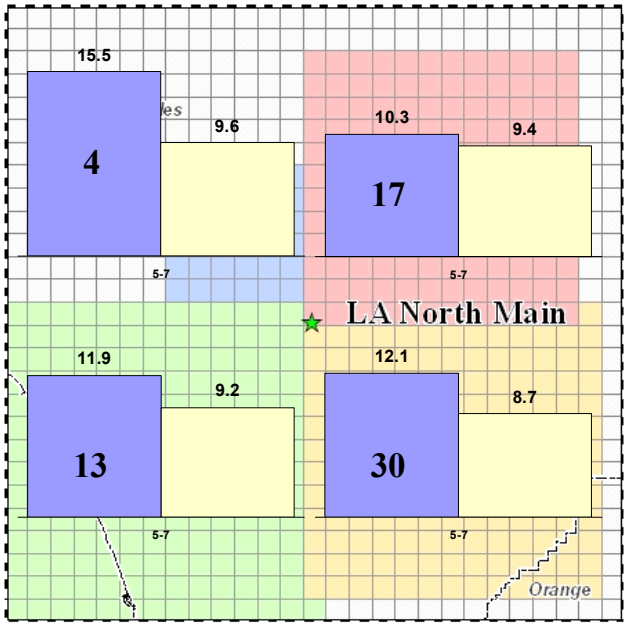
Los Angeles North Main ambient- and EI-derived ratios for 0500-0700 PST, 2001 (full analysis zone extent)

Discussion of Potential Analyses (3 of 6)

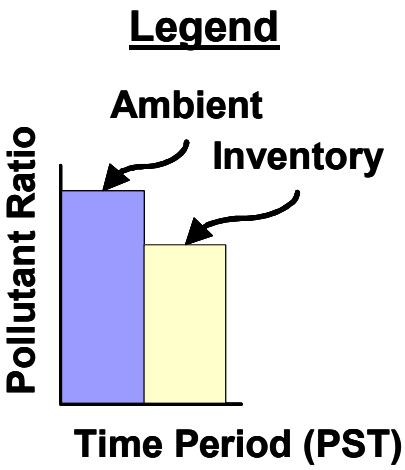
EI Reconciliation with Pollutant Ratios



PAMS HC/NO_x



CO/NO_x



Los Angeles North Main ambient- and EI-derived ratios by wind quadrant for 0500-0700 PST, 2001

Discussion of Potential Analyses (4 of 6)

EI Reconciliation with Speciated VOCs

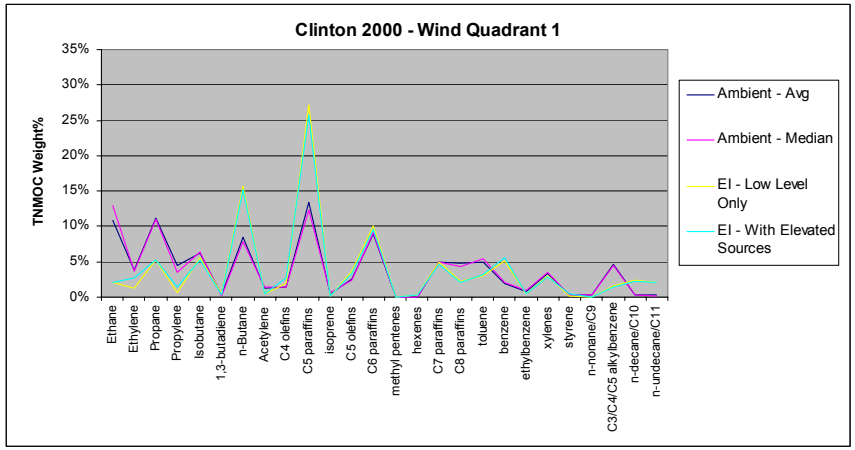
	Acetylene/ Benzene		Ethylene/ Acetylene		Benzene/ Xylene		Benzene/ Toluene		CO/Benzene		Isoprene/ PAMSHC		Total Aromatics/ PAMSHC	
Site	EI	Amb	EI	Amb	EI	Amb	EI	Amb	EI	Amb	EI	Amb	EI	Amb
All	0.97	1.50	2.12	1.53	0.34	0.36	0.25	0.26	174.8	185.4	0.0011	0.0021	0.217	0.182
WD 1	1.00	1.55	2.08	1.57	0.34	0.36	0.26	0.27	182.5	185.0	0.0011	0.0019	0.217	0.191
WD 2	0.92	1.48	2.14	1.57	0.35	0.36	0.24	0.25	170.3	185.4	0.0010	0.0022	0.221	0.182
WD 3	0.99	1.67	2.13	1.43	0.34	0.35	0.25	0.26	169.4	180.0	0.0011	0.0021	0.216	0.180
WD 4	1.00	1.38	2.07	1.64	0.34	0.36	0.27	0.30	180.7	220.8	0.0011	0.0025	0.211	0.196

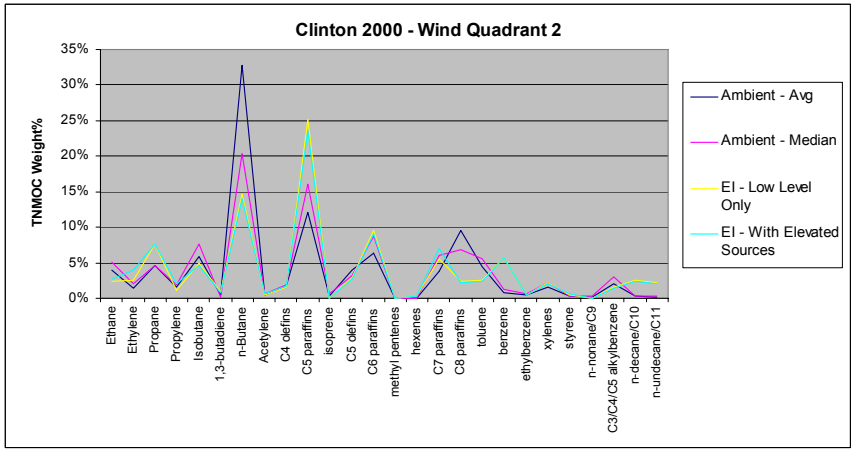
Note: WD = wind direction

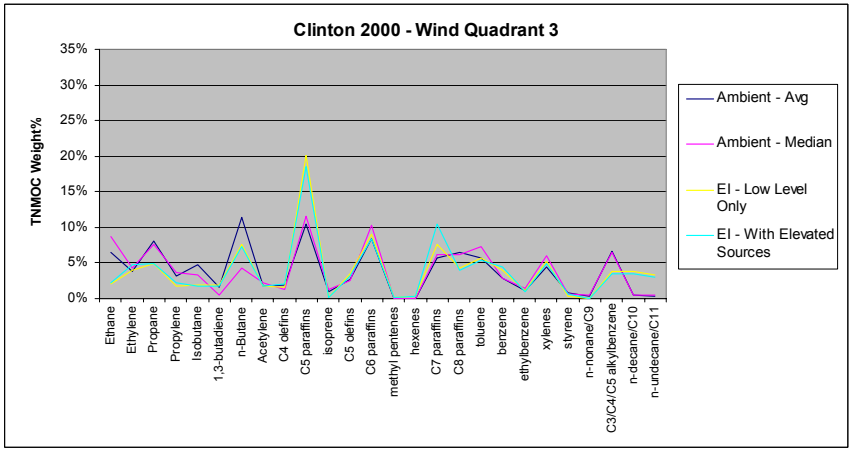
Los Angeles North Main EI/ambient species ratio comparison for weekdays in 2001

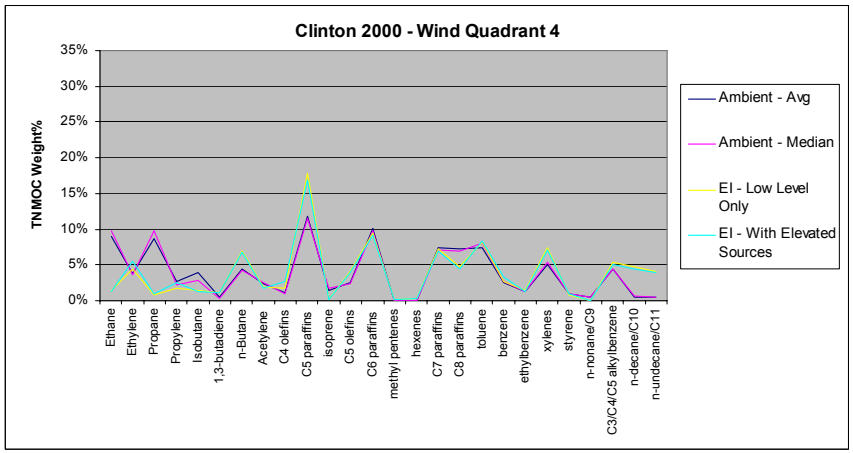
Discussion of Potential Analyses (5 of 6)

EI Reconciliation with Speciated VOCs





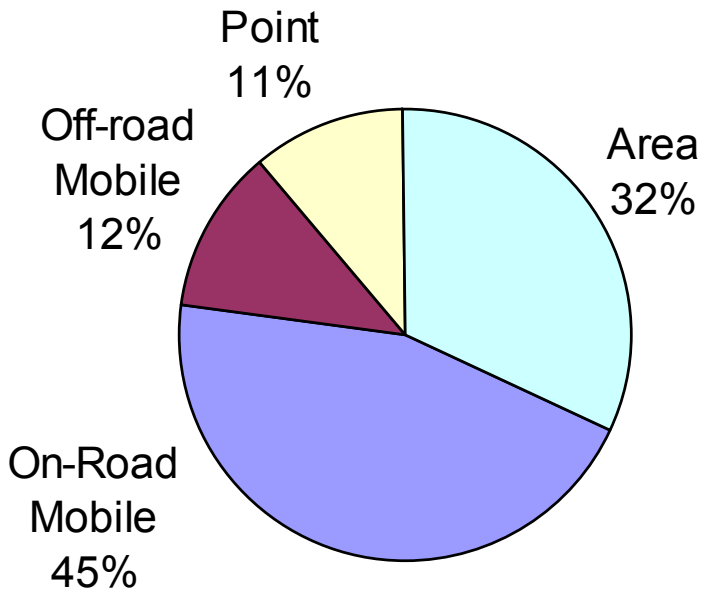




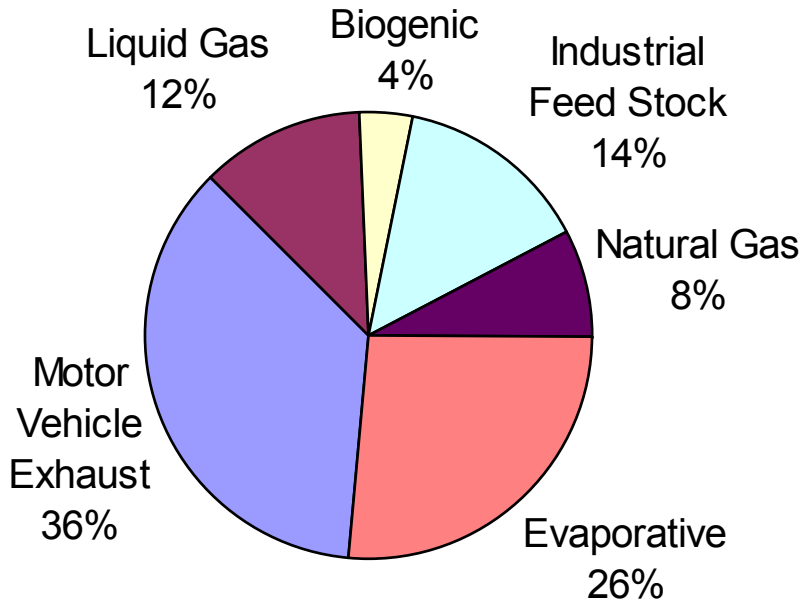
Comparison of ambient- and EI-derived TNMOC compositions by wind quadrant for the Clinton site in 2000 (Houston area)

Discussion of Potential Analyses (6 of 6)

Hawthorne (SoCAB) TNMOC Composition, 0500-1000 PST



By EI Category



By Source Apportionment Factor

Review and Recommendations (1 of 2)

- Assess sources of uncertainty or bias
  - How representative is monitoring data for assessing nearby emissions (transport issues, etc.)?
  - What are the underlying assumptions of analysis methods used and their impacts on the conclusions?

Review and Recommendations (2 of 2)

- Synthesize Findings
  - Formulate overarching conclusions
  - Summarize the apparent strengths and weaknesses of the EI
  - Make recommendations for "corroborative adjustments" to the EI

Project Schedule

Task	Deliverables	Due Date
All	Progress reports and invoices	Monthly
1	Project kickoff meeting	October 20, 2005
1	Draft work plan	October 27, 2005
1	Final work plan	November 10, 2005
2	Draft technical memorandum (air quality data availability)	November 30, 2005
2	Final technical memorandum (air quality data availability)	December 9, 2005
3	Draft technical memorandum (speciation review)	November 30, 2005
3	Final technical memorandum (speciation review)	December 9, 2005
4	Task 4 workshop	December 14, 2005
4	Draft technical memorandum (alternative data analysis methods)	January 16, 2006
4	Final technical memorandum (alternative data analysis methods)	February 1, 2006
All	Provide interim results to the extent possible	As available
11	Draft interim report	March 15, 2006
11	Draft final report, manuscript, software, data files, and documentation	June 15, 2006
11	Final report and manuscript	August 15, 2006